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Tunneling spectroscopy of nonequilibrium interacting impurity states on semiconductor surface

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Abstract. New STM/STS observation method has been used for investigation of interacting nonequilibrium impurity states on semiconductor surface. The dependence of electronic density spatial distribution on applied tunneling voltage is analyzed. Energy values of "switching on and off" of interatomic interactions are determined. The dependence of Cr impurity dangling bond hybrid orbital electron spatial localization on tunneling bias is observed.

In present work we report the results of STM/STS investigations of interacting nonequilibrium impurity states on A_3B_5 semiconductor surface. Images of tunneling conductivity spatial distribution on semiconductor surface have been obtained by means of new observation method. The series of images has been consequently measured step by step changing applied tunneling bias (energy of electronic states) by 5 mV. The dependence of electron density spatial distribution in the vicinity of interacting impurity atoms upon applied bias voltage (the energy of electronic states) has been investigated by STS method.

Monocrystal GaAs Si doped samples and double doped samples with Si and Zn impurities (copmensated) have been used in our experiments. All the measurements were performed at $T \sim 4$ K using low temperature STM with sample cleavage mechanism [1].

The evolution of local electronic density spatial distribution of interacting impurities with energy changing is depicted in Fig. 1. Changes in spatial configuration of different impurity atoms overlapping electronic states with energy variation are quite visible on series of $dI/dV(V, X, Y)$. Analyzing spatial distribution of tunneling conductivity one can follow symmetry properties of electronic states with different energies and also determine characteristic energy values of "switching on and off" of interatomic interaction.

Electronic density spatial structure measured in the vicinity of two interacting impurities at fixed value of applied bias voltage is sensitive to symmetry properties of localized state with definite energy which can be determined from applied tunneling voltage value. We should mention the main specific features observed in tunneling conductivity spectra:

1. Peaks on tunneling conductivity spectra $dI/dV(V, X, Y)$ are clearly seen just above interacting impurity atoms and disappear if the distance from impurities exceeds the maximum value of localization radius for interacting impurities localized state (for "shallow" impurities it is about 10 nm). Peaks structure on tunneling conductivity curves strongly depends on type of impurity and interatomic interaction. With increasing of the distance from impurities not only peaks intensity changes but its maximum energy also shifts. This fact can be connected with strong influence of Coulomb interaction of localized impurity charges on electronic energy spectrum.
2. Characteristic energy range of considerable changes in local electronic density distribution is about 0.1 eV. This value is comparable with localized state energy broadening due to manyparticle interaction. Theoretical analyzis of energy spectrum and symmetry

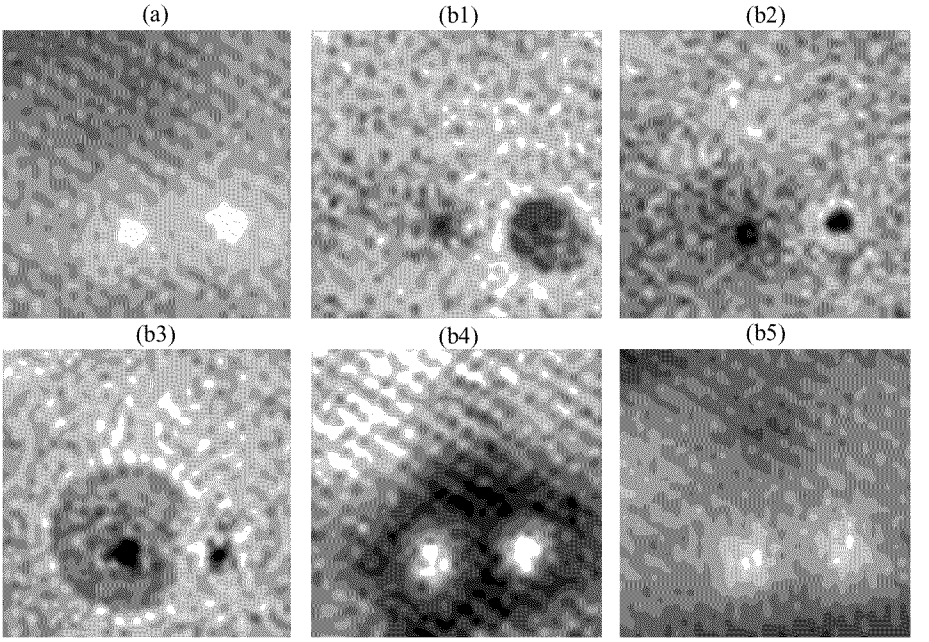

Fig. 1. Evolution of local electron density distribution (LEDD) of two interacting impurity Si atoms with tunneling sample bias (energy) changing: (a) STM image Si–Si, $U_t = 1.0$ V, (b) LEDD images Si–Si, U_t from 1.0 V to -1.5 V, (images size 10 nm $\times$ 10 nm).

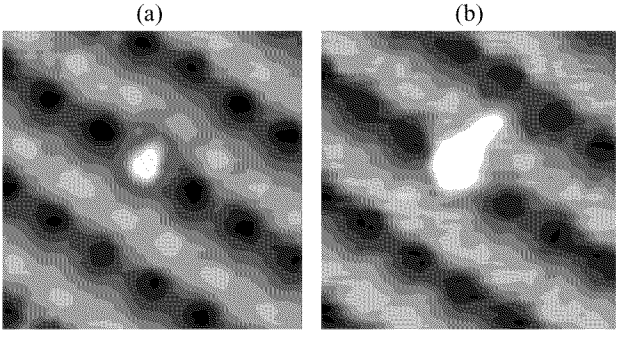

Fig. 2. The dependence of Cr impurity hybryd orbital localization on applied tunneling sample bias: (a) $U_t = -1.0$ V, (b) $U_t = -1.1$ V.

properties of different electronic states in two-site extended Hubbard model gives qualitative explanation of main specific features experimentally observed in local tunneling conductivity spectra.

Interacting impurity states of Cr atom on InAs (110) surface have been also investigated by STS/STM methods. Such states appear due to substitution of As site by Cr atom in InAs lattice. Effects of resonant tunneling for these impurities were observed earlier [2]. The dependence of Cr impurity atom dangling hybrid orbital spatial localization on applied tunneling voltage is shown in Fig. 2. It is clearly seen, that Cr atom occupies As site and impurity perturbation potential radius is limited by crystal lattice unit cell. Shape of enhanced electron density near impurity atom corresponds to spatial localization of Cr

dangling bond hybrid orbital unpaired electron when "upper" In atom is absent due to crystal cleavage. Directed shape of hybrid orbital with characteristic size ~0.5 nm points to the presence of d-electron state [3]. Estimation of Coulomb repulsion energy U for localized electrons in Hubbard model yields $U \sim e^2/a_0 \sim 0.5$ eV if $a_0 \sim 0.5$ nm. This value is comparable with band gap width. So STS spectra shift occurs in the vicinity of impurity state.

Analyzing the results of STS/STM investigations of different impurities we have found out some general similarities in behaviour of their STS/STM images and tunneling conductivity spectra. We have also examined fundamental physical effects responsible for specific features of tunneling spectra and changes in STM/STS images near atomic impurities of different types [4]. So it become possible to identify single atomic impurity in semiconductor matrix.

We should also mention that unique method firstly used here for registration of evolution of electronic density spatial distribution can be also applied for control and modification of information bit (Q-bit) states, based on individual interacting impurity atoms in semiconductor matrix [5].

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